MST eNEWS

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INSIDE

Polish science and technology university recognizes Zurek for materials science contributions

In a gala ceremony on May 11, Materials in Radiation and Dynamic Extremes (MST-8) Group Leader Anna Zurek was awarded a medal of appreciation for her contributions to materials science and metallurgy and many years of fruitful international collaboration between AGH University of Science and Technology in Krakow, Poland and Los Alamos National Laboratory.

Zurek's efforts have led to collaborations between MST-8 staff and students, postdocs, and faculty of the university (especially with Prof. dr hab. inz. Janusz Majta), including two appointments for a long-term visiting scientist. These collaborations have resulted in several PhD theses, a doctoral habilitation thesis, the Maria Sklodowska–Curie International (Polish-American) research Fund II Award (in 1997-2000), and 29 collaborative research papers on the subject of characterization and modeling of materials deformed under extreme, dynamic conditions.

Zurek, who joined Los Alamos in November 1985 in (then) MST-5, earned her MS in the Materials Science and Metallurgy Department from the University of Science and Technology, Krakow, in 1976 and her PhD in materials science from the University of Texas at Austin in 1981.

Above: Anna Zurek being presented with a medal of appreciation by Prof. dr hab. inż. Tadeusz Słomka newly elected, incoming rector of the university. Left: Zurek is joined by other medal recipients at the university event. Right: Close up of the medal.

Change of management in MST-8

In April's edition of "From the Desk," Mark Bourke talked about the breadth of applied and fundamental studies of radiation effects in MST Division. As I write this column today, Mark has been chosen and promoted to the position of Lujan Center Leader. Mark was the MST-8 deputy group leader for 9 years and I want to thank him for his contributions and dedication to the group. I also am hoping for the continued, successful, and close collaboration between the Lujan Center and MST in the years to come.

In the meantime, Stu Maloy has graciously agreed to serve as acting deputy group leader. With Stu's appointment we aim to have leadership continuity in the area of materials science under extreme radiation conditions. He has long-term connections and leadership experience with DOE- supported nuclear energy programs and is presently the core materials technical lead with the DOE Fuels Cycle Research and Development program. Stu has contributed to many projects related to our group's mission, bridging the knowledge between both sides of the group—the materials under radiation extremes as well as working on materials under dynamic deformation conditions. Stu's unique talents and leadership skills are very welcome and I am very happy and excited to introduce him as our new acting deputy group leader.

Celebrating success

A couple of weeks ago I returned from a vacation visiting with my family and friends in Poland. I planned this trip many months in advance and was surprised at the last minute (one day before the departure) to be invited to participate in the 90th anniversary celebration of the Metals Engineering and Industrial Computer Science Department at the University of Science and Technology in Krakow. This was my alma matter department, where I received my MS degree. What surprised me the most was the ceremonial gallantry, pageantry, tradition, and size of the celebratory production—something that I have not experienced since I came to the United States in 1976! It was a memorable event and experience for me. It made me think about how we really remember the passing of time. How do we really measure time? In our personal lives we remember the year we graduated, got married, or years of births of our children, and hopefully anniversaries. In our professional lives, we measure time by when we got the special job we so badly wanted, by the year of promotion, by a first paper that was particularly difficult to publish in a journal, by the grant we received, by the complicated milestone achieved, or by a discovery we just made.

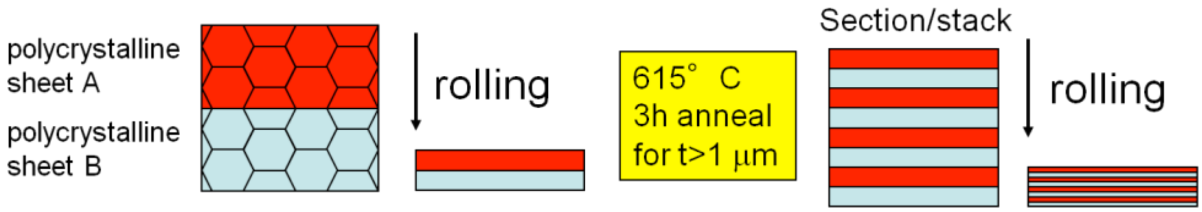
'I would love to encourage each of you to reach out to your employees and colleagues with a word of encouragement about the hard work that they are doing.'

What I have observed in the most recent years is that we as a Laboratory tend to measure time by the incidences in safety and security. Although it is very important to remember those in order not to repeat our mistakes and to learn from them—as managers we frequently forget to celebrate our employees' successes. This is more important now than ever, considering that during a time of austerity, financial shortages, and economic problems, scientific accomplishments and /or milestone deliverables are difficult to achieve. We need more encouragement and celebrations of success in order to build up the morale of our employees.

With this said, I would love to encourage each of you to reach out to your employees and colleagues with a word of encouragement about the hard work that they are doing.

Thank you all for your hard work during difficult times and congratulations on your achievements!

— MST-8 Group Leader Anna Zurek



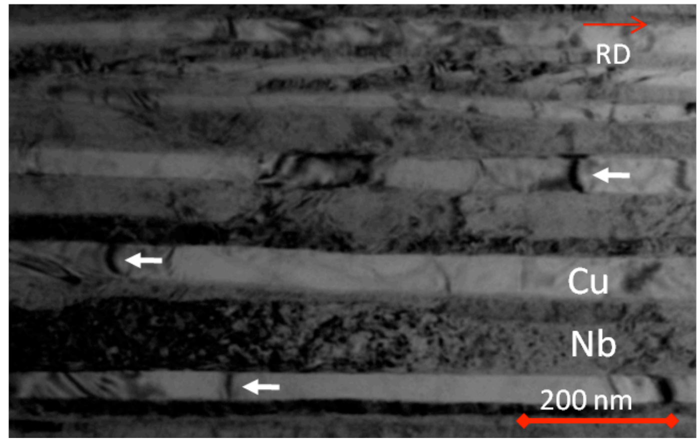


Figure 1 (above): Schematic of the accumulative roll bonding process. Figure 2 (right): Bright Field TEM image of ARB Cu-Nb nanolamellar multilayers with individual layer thicknesses of 48 nm. Red arrow indicates rolling direction and white arrows indicated evidence of confined layer slip.

Bulk texture evolution of nanolamellar composites during accumulative roll bonding

In bulk multi-phase composite metals containing an unusually high density of heterophase interfaces, the bi-metal interface controls all defect-related processes. Quite unconventionally, the constituent phases play only a secondary role. With the "right" characteristics, these bi-material interfaces can possess significantly enhanced abilities to absorb and eliminate defects. Through their unparalleled ability to mitigate damage accumulation induced under severe loading and/or severe environments, they provide their parent composite with a highly effective healing mechanism and an unrivaled robustness not possible in existing advanced structural materials.

Atom-by-atom fabrication of copper-niobium (Cu-Nb) nanolamellar composites prepared via physical vapor deposition (PVD) exhibit orders-of-magnitude increases in desirable properties such as strength, resistance to radiation damage, resistance to shock damage, and thermal stability when compared with their bulk counterparts. Modeling indicates that the desired properties of the nanolamellar composites are tied to the specific atomic structure that is exhibited at the interfaces between the two materials. The atomic structure of PVD Cu-Nb promotes recombination and annihilation of defects leading to a self- healing interface. These unique properties make the material attractive for nuclear power, transportation, energy, and defense applications. Los Alamos researchers and a collaborator have investigated scalable fabrication methods that can produce bulk material (as the potential applications require) that are geometrically similar to PVD multilayers but with different interfacial structures. Having a different interfacial structure would allow researchers to distinguish the effect of the high density of heterophase interfaces from the interfacial structure in determining the desirable properties listed above. The journal *Acta Materialia* published the research.

The researchers examined accumulative roll bonding (ARB) as a scalable method to fabricate Cu-Nb composites that are geometrically similar to those produced by the physical vapor deposition method. The ARB process begins with two 1 mm thick plates of fully annealed, high purity Cu and Nb as shown in Figure 1. A pass with a 60% reduction in overall thickness is made through a rolling mill to induce bonding between the two stacked plates. After the pass is performed, the new, single plate is cut, restacked, and sent through the mill on another 60% reduction pass. This process is repeated with intermittent annealing steps to offset the differences in work hardening between Cu and Nb. The scientists successfully manufactured bulk sheets of Cu-Nb multilayer composites with more than 14,000 layers and individual layer thicknesses as small as 10 nm.

Because the ARB Cu-Nb has a layered morphology similar to PVD Cu-Nb, the researchers conducted a bulk texture study at the Lujan Neutron Scattering Center to examine the evolution of the interfaces from the ARB process. The scientists found that the interfaces in ARB Cu-Nb evolve towards an atomic structure that is fundamentally different from that exhibited in PVD due to the extreme strain infused during the ARB process. White arrows in Figure 2 indicate where confined layer slip, a deformation mechanism, is observed. Confined layer slip was observed in the PVD Cu-Nb system at this same layer thickness. This finding indicates that the same deformation mechanisms are present and active despite the difference in fabrication and interfacial structure.

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Texture . . . Now the researchers are determining how the difference in interfacial structure of Cu-Nb affects thermal stability, radiation damage resistance, strength, and shock resistance. John Carpenter and Duncan Hammon (Materials Technology-Metallurgy, MST-6), Nathan Mara (Center for Integrated Technologies, MPA-CINT), Irene Beyerlein (Fluid Dynamics and Solid Mechanics, T-3), Sven Vogel (Lujan Neutron Scattering Center, LANSCE-LC), and Jonathan LeDonne (Carnegie Mellon University) conducted the research. Reference: "Bulk Texture Evolution of Cu–Nb Nanolamellar Composites during Accumulative Roll Bonding," *Acta Materialia* **60**, 1576 (2012).

The Laboratory Directed Research and Development (LDRD) program funded the research, and the DOE Office of Basic Energy Sciences sponsors the Lujan Neutron Scattering Center at LANSCE. The work supports the Lab's Energy Security and Global Security mission areas and the Materials for the Future science pillar.
Technical contact: John Carpenter

ICE II experiment furthers understanding of irradiation effects on LBE-induced corrosion on steel

Research benefits advanced nuclear reactor concepts

Lead bismuth eutectic (LBE) is a leading candidate for use as a coolant in some advanced nuclear reactor concepts as well as in spallation neutron sources such as the Materials Test Station proposed for operation at the Los Alamos Neutron Science Center (LANSCE). It has excellent thermal properties, high neutron yield, and low melting point (123 °C). However, one challenge is that at typical operating temperatures, which can be as high as 500°C, it is modestly corrosive to some steels including HT-9 ($Fe_{84.36}Cr_{11.9}4$ $Ni_{0.62}W_{0.48}Mo_{1.03}Mn_{0.69}Si_{0.30}V_{0.30}C_{0.21}$ and trace amounts of S, P, Cu, Co, N, Al, and Ti in wt%), which is the leading candidate for many applications. The corrosion effects have been extensively studied without concomitant radiation, but one major question is whether the addition of a radiation environment impedes or accelerates the corrosion process (theories advocate each possibility).

To explore that question researchers from MST-8 and from the University of California, Berkeley designed an experiment to expose a thin window of HT-9 in contact with molten LBE at 430 °C to a 5.5-MeV proton beam. The window thickness and beam energy were chosen to maximize the irradiation damage at the contact layer between the LBE and the HT-9. The goal was to examine whether the oxide formed in the region exposed to the ion beam differed in nature or rate of formation from oxide formed without the presence of ion beam damage.

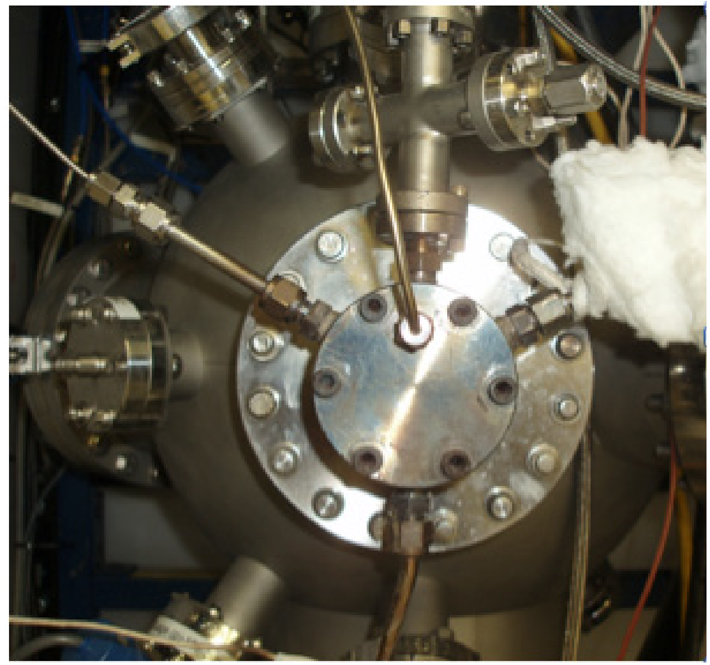

Figure 3 (above) Irradiation and Corrosion Experiments chamber; and (below) LBE corrodes through HT-9 concave shaped disk after 60 hours irradiation with 5.5 MeV protons to an accumulated dose of 3.8 dpa.

The experiment is referred to as ICE-II (irradiation and corrosion experiment) and builds on ICE-I, which was the first attempt to perform this study. The ICE-I experiment was reported in 2008 (*J. Nucl. Mat.* **376** (2008)). ICE–II builds on the first experiment by allowing higher temperature and includes the ability to monitor oxygen content (which is a crucial factor controlling the rate of corrosion). Improvements in the shielding enabled higher beam flux, longer duration irradiations, and thus higher dose. During a 60-hour irradiation approximately 4 displacements per atom (dpa) were induced at the surface contacting LBE and metal.

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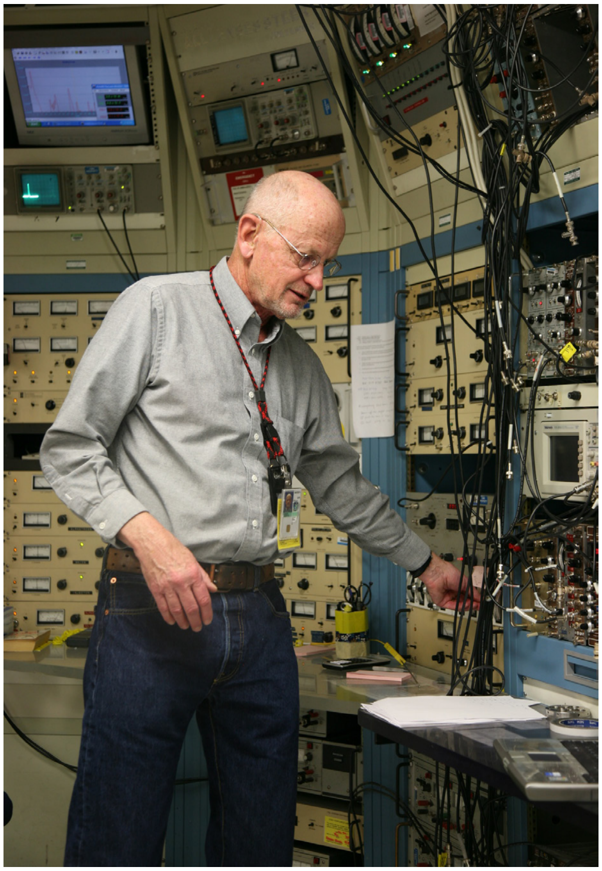

Joe Tesmer oversees operations during the experiment.

ICE II . . The corrosion apparatus was designed and built by Staffan Qvist and Peter Hosemann (UC Berkeley). Magda Caro, Yongqiang Wang, Joseph Tesmer, John Balog, and Mark Bourke (all MST) integrated the capability onto the tandem accelerator in the ion beam materials laboratory (IBML). The chamber is shown in Figure 3.

The experiment demonstrated that multiday corrosion/irradiation studies are possible in the IBML.

Preliminary post irradiation characterisation revealed a possible synergistic effect of radiation and corrosion. Notably the sample failed sooner than was expected and close examination of Figure 3 shows a penetration at the center of the concave-shaped HT-9 thin window after 60 hours irradiation. This was unexpected. Preliminary SEM studies indicate a difference between the irradiated and non-irradiated regions. Detailed microstructural analysis is ongoing.

John Bliss (Radiation Protection Technical Support, RP-3) helped with MCNPX dose calculations. Antonio Maestas and Rebekkah Aguilar (RP-1) helped with radiation monitoring. Engang Fu and Carol Haertling (both at MST) helped performing ion irradiation. The research was funded by the Laboratory Directed Research and Development (LDRD) program.

Technical Contacts: Yongqiang Wang and Magda Caro

HeadsUP!

New website for ADEPS Worker Safety and Security Team

The ADEPS WSST has a resource and information page located on the ADEPS internal website:

int.lanl.gov/org/padste/adeps/wsst.shtml

The site includes the team's most recent meeting minutes as well as links to a wide range of related safety and security information.

Your ADEPS WSST members are

- ADEPS: Jeff Schinkel
- LANSCE-DO: Howard Nekimken
- LANSCE-LC: Eric Larson
- MPA-CMMS: Michael Torrez
- MPA-MC: Eve Bauer, chair
- MST-6: Erik Luther
- MST-8: Thomas Sisneros
- P-25: Jeff Bacon, co-chair

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries this month:

John Kennison, MST-6	20 years
Carol Haertling, MST-6	15 years
Hunter Swenson, MST- 6	10 years
Karl Krenek, MST-16	10 years
Jung Rim, MST-7	5 years

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To submit news items or for more information, contact Karen Kippen, EPS Communications, at 606-1822, or kkippen@lanl.gov.

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Nonadiabatic forces in ion-solid interactions: The initial stages of radiation damage

Nuclear reactions produce highly energetic ions that can travel long distances in matter. When one of these fast ions traverses a material, it loses energy due to atomic and electronic collisions, producing damage.

At high projectile energies the main dissipation mechanism is friction with the electrons, which follow the rules of quantum mechanics. Like a speedboat in a calm lake, the passage of the fast ions creates a disturbance, in the shape of a wake, of the electron density.

In a new research Alfredo Caro (MST-8), together with colleagues from Lawrence Livermore National Laboratory, United Kingdom, and Spain, simulated this quantum friction of the electrons to calculate for the first time the connection between nuclear and electronic stopping cross section. This is possible because the simulation took into account the individual dynamics of the electrons in an approach known as Ehrenfest dynamics.

The team simulated the passage of a proton in crystalline aluminum. By accounting how much energy is absorbed by the electrons and how much impulse is given to the rest of the atoms, the team predicted how the inter-atomic interactions are altered by the excitation of the electrons. This is a precise measure of how much damage energy is deposited into the material. The figure at right that appears on the cover of *Physical Review Letters*, represents this wake.

The new method allows predicting the behavior of complex materials under the effect of radiation. A full understanding of these early stages of radiation damage provides knowledge and tools to manipulate them to our advantage. This understanding not only applies to materials for nuclear applications, but also for materials related to the space industry, novel processing techniques using lasers and ions, in biology and medicine, including the large field of assessing the effects of radiation on living tissues, both for understanding damage and for therapeutic use such as cancer-therapy conducted by charged particles.

Model of the electronic wake (blue surfaces) generated by an energetic proton (red sphere) traveling in an aluminum crystal. The resulting change in electronic density is responsible for modification of chemical bonds between the atoms and consequently for a change in their interactions. [Alfredo A. Correa, Jorge Kohanoff, Emilio Artacho, Daniel Sánchez-Portal, and Alfredo Caro, Phys. Rev. Lett. ***108****, 213201 (2012)].*

This new simulation capability constitutes a first step towards a unified method of simulation of the electron and atom dynamics beyond the Born-Oppenheimer approximation, so far a keystone of molecular dynamics simulation of radiation damage.

The research appeared in *PRL* **108**, 213201 (2012) (Alfredo A. Correa Lawrence Livermore National Laboratory, Jorge Kohanoff Queen's University, Belfast UK, Emilio Artacho University of Cambridge UK, Daniel Sanchez-Portal Sebastian, Spain; Alfredo Caro, Los Alamos National Laboratory, "Nonadiabatic forces in ion-solid interactions: The initial stages of radiation damage."